

ABSTRACT

A three-dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.